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Quasi-steady-state approximation for a reaction–diffusion system with fast intermediate

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ABSTRACT

We consider a prototype reaction–diffusion system which models a network of two consecutive reactions in which chemical components A and B form an intermediate C which decays into two products P and Q. Such a situation often occurs in applications and in the typical case when the intermediate is highly reactive, the species C is eliminated from the system by means of a quasi-steady-state approximation. In this paper, we prove the convergence of the solutions in L^2, as the decay rate of the intermediate tends to infinity, for all bounded initial data, even in the case of initial boundary layers. The limiting system is indeed the one which results from formal application of the QSSA. The proof combines the recent L^2-approach to reaction–diffusion systems having at most quadratic reaction terms, with local L^∞-bounds which are independent of the decay rate of the intermediate. We also prove existence of global classical solutions to the initial system.

1. Introduction and main results

Mathematical models of chemically reacting real systems (e.g., combustion, atmosphere chemistry, industrial processes) usually consist of tens of chemical species involved in a large number of chemical reactions. This leads to complex reaction networks which often require massive simplifications due to several reasons. First, many of the occurring species are actually intermediates which are formed by one or a few reactions and are immediately consumed in consecutive ones. Such species are often highly reactive and, hence, only exist in trace quantities – sometimes these species cannot even be detected nor measured. In such situations models are needed which do not include these intermediate chemical components. Second, even if the full mechanism with all intermediates and elementary reaction steps is known, rate constants for the individual steps are often unavailable. This is in particular true for the very fast decay of highly reactive intermediates. Hence, simplified reaction mechanisms with only few species, formal reactions and rate laws/constants are again required. Third, the appearance of a wide range of time scales for the different chemical reactions leads to systems of either ODEs (in the ideally mixed homogeneous case) or PDEs which are extremely stiff and therefore expensive in their numerical solution.

Simplifications of large reaction networks are done routinely in Chemical Engineering, although mathematical proofs are often missing. There are two well-known approaches which apply in different cases: if the network contains a set of reversible reactions which are much faster then the remaining ones, a quasi-steady-state approximation with respect to the fast reversible reactions is done. This "projects" the system onto a limiting manifold on which all fast reactions are at equilibrium. For the ODE-case of homogeneous systems, this method is reviewed in [15]. A rigorous result concerning the passage to the corresponding limit system is given in [8]; cf. also the references given in [15]. Rigorous results for reaction–

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diffusion systems are missing. We are only aware of [9], where the simplest case of a single reversible reaction of type $mA \rightleftharpoons nB$ with mass action kinetics is considered.

The second approach for model reduction applies to systems with highly reactive intermediates. Here, a quasi-steady-state approximation is done with respect to these "fast" species, by formally setting their rate of change to zero. This leads to algebraic expressions which are used to eliminate the concentrations of these intermediates. Sometimes this approach is also called pseudo-steady-state hypothesis, Bodenstein's method or method of adiabatic elimination. For more details on this method applied to chemically reacting homogeneous systems we refer to [12] and [13]. The Bodenstein method is also mostly applied without rigorous justification, even in situations where transport processes like convection or diffusion need to be modeled as well.

We are therefore interested in a rigorous analysis of the instantaneous limit of reaction–diffusion systems with fast intermediates. In the present paper we consider the following prototype reaction network composed of two consecutive reversible chemical reactions:

$$A + B \rightleftharpoons C \rightleftharpoons P + Q.$$

Here the intermediate species C is viewed as a transition complex which is highly unstable, i.e. the decay of C into the products P and Q or back to the educts A and B is extremely fast. According to the mass action law and assuming that the whole system is isolated, we obtain the following system of reaction–diffusion equations:

$$\begin{cases} \left.\begin{array}{l} \partial_t a - d_a \Delta a = -k_1 ab + k_2 c \\ \partial_t b - d_b \Delta b = -k_1 ab + k_2 c \\ \partial_t c - d_c \Delta c = k_1 ab - k_2 c - k_3 c + k_4 pq \\ \partial_t p - d_p \Delta p = -k_4 pq + k_3 c \\ \partial_t q - d_q \Delta q = -k_4 pq + k_3 c \end{array}\right\} \quad \text{on } (0,+\infty) \times \Omega, \\ \partial_n a = \partial_n b = \partial_n c = \partial_n p = \partial_n q = 0 \quad \text{on } (0,+\infty) \times \partial\Omega, \\ a(0,\cdot) = a_0, b(0,\cdot) = b_0, c(0,\cdot) = c_0, p(0,\cdot) = p_0, q(0,\cdot) = q_0. \end{cases} \tag{1}$$

Here a, b, c, p, q denote the molar concentrations of the reacting species, the d_j $(j = a, b, c, p, q)$ are positive diffusion coefficients, k_i $(i = 1 \ldots 4)$ are positive rate constants and a_0, b_0, c_0, p_0, q_0 are the initial concentrations which we assume to be nonnegative and bounded. Finally, Ω is a given bounded open subset of $\mathbb{R}^N$ with sufficiently smooth boundary ($\partial\Omega \in C^{2+\epsilon}$, say) and ∂_n denotes the outer normal derivative to $\partial\Omega$.

As mentioned above, we are mainly interested in what happens to the solutions of this system when the life-time of the complex C is very short, or, in other words, when the rate constants k_2, k_3 tend to $+\infty$. The same question has recently been studied in [5], where first convergence results have been obtained in case of zero initial intermediate concentration. Our result is stronger in several respects: more details are given at the end of this introduction after the statement of our main results.

Let us note in passing that the above system of consecutive reactions is very close to the standard enzyme-substrate reaction mechanism of Michaelis–Menten,

$$E + S \rightleftharpoons C \to E + P,$$

in which an enzyme reacts with the substrate to form a complex which then decays to the product; here the enzyme acts as a catalytic substance, i.e. it is not consumed by the reaction. For this particular system, an interesting review and extension of the quasi-steady-state approximation in the homogeneous (ODE-)case is given in [29], while different quasi-steady-state approximations for different relations between the time scales of reactions and diffusion are (formally) derived in [20] in case of one spatial dimension.

Local existence in time of nonnegative solutions to (1) is classical for given nonnegative and bounded initial data (see Lemma 7 in Appendix A). However, global existence for $t \in [0,+\infty)$ is not straightforward. *We first prove here that global classical solutions do exist* by adapting the L^p-duality technique developed in [19,22,23,14].

We will throughout assume

$$d_a, d_b, d_c, d_p, d_q > 0, \qquad k_1, k_2, k_3, k_4 > 0, \qquad a_0, b_0, c_0, p_0, q_0 \in L^\infty(\Omega; \mathbb{R}_+). \tag{2}$$

We prove the following global existence result where, by *classical solution*, we mean that

$$\forall T > 0, \quad a, b, c, p, q \in C^2\big((0,T] \times \overline{\Omega}\big) \cap L^\infty\big((0,T) \times \Omega\big) \cap C\big([0,T]; L^1(\Omega)\big), \tag{3}$$

and that (1) is satisfied in a classical sense.

Theorem 1. *Assume* (2)*. Then the system* (1) *has a unique global classical nonnegative solution.*

Now, to study the limit of instantaneous decay of the intermediate, we assume

$$k := k_2 + k_3 \to +\infty, \qquad \frac{k_2}{k_2+k_3} \to \alpha \in [0,1], \qquad \frac{k_3}{k_2+k_3} \to \alpha' := 1-\alpha. \tag{4}$$

We prove the following result:

Theorem 2. *Assume* (2) *and* (4). *Then, up to a subsequence, the solution* $U_k = (a_k, b_k, c_k, p_k, q_k)$ *of* (1) *converges in* $L^2(\Omega)^5$ *to* $U = (a, b, 0, p, q)$, *where* (a, b, p, q) *is a* weak solution *on* $[0, +\infty)$ *of*

$$\begin{cases} \left.\begin{array}{l} \partial_t a - d_a \Delta a = -\alpha' k_1 ab + \alpha k_4 pq \\ \partial_t b - d_b \Delta b = -\alpha' k_1 ab + \alpha k_4 pq \\ \partial_t p - d_p \Delta p = \alpha' k_1 ab - \alpha k_4 pq \\ \partial_t q - d_q \Delta q = \alpha' k_1 ab - \alpha k_4 pq \end{array}\right\} \quad \text{on } [0,+\infty) \times \Omega, \\ \partial_n a = \partial_n b = \partial_n p = \partial_n q = 0 \quad \text{on } (0,+\infty) \times \partial\Omega, \\ a(0,\cdot) = a_0 + \alpha c_0, b(0,\cdot) = b_0 + \alpha c_0, p(0,\cdot) = p_0 + \alpha' c_0, q(0,\cdot) = q_0 + \alpha' c_0. \end{cases}$$

Note that the original initial value for finite k_2, k_3 is in the limit projected onto the manifold $\{c = 0\}$ in such a manner that the quantities $a - b$, $p - q$ and $a + b + 2c + p + q$ are conserved.

Here, by *weak solution*, we mean that for all $T > 0$ and $Q_T = (0, T) \times \Omega$,

$$a, b, p, q \in L^2(Q_T) \cap C\big([0,T]; L^1(\Omega)\big) \cap L^1\big((0,T); W^{1,1}(\Omega)\big), \tag{5}$$

and for all $\psi \in C^\infty([0,T] \times \overline{\Omega})$ with $\psi(T) = 0$ we have

$$-\int_\Omega \psi(0)(a_0 + \alpha c_0) + \int_{Q_T} -\partial_t \psi a + d_a \nabla\psi \nabla a = \int_{Q_T} \big(-k_1 \alpha' ab + k_4 \alpha pq\big)\psi, \tag{6}$$

and similarly for the other components b, p, q. Note that the nonlinear terms ab, pq are in $L^1(Q_T)$ since all components are in $L^2(Q_T)$. Since all components belong to $L^1(0, T; W^{1,1}(\Omega))$ (see more comments on this space in Appendix A), it follows that $\nabla a \in L^1(Q_T)$ and similarly for $\nabla b, \nabla p, \nabla q$. Therefore, Eq. (6) does make sense. Here, the Neumann boundary data are to be understood in a weak sense; more details are given in Appendix A about weak solutions.

Our main contribution here concerns the convergence result itself. Global existence of weak solutions is not new for the limit system itself (see [25,11]). Local existence of classical solutions is well-known, but *existence of global classical solutions is an open problem* (except for $\alpha = 0$ or $\alpha = 1$, see below). The believed conjecture is rather that, in general, L^∞-blow up does occur in finite time as proved for similar systems in [26,27]. More precisely, it is proved in [16] that solutions are indeed classical in dimensions $N = 1$ and $N = 2$. In the same paper [16], it is proved that for $N = 3, 4$, the Hausdorff dimension of the set of the possible blow-up points in $(0, +\infty) \times \Omega$ is bounded above by $(N^2 - 4)/N$. It is not known whether this estimate is optimal or not.

Note that for $\alpha = 0$ (resp. $\alpha = 1$), we obtain an irreversible reaction in the limit, namely

$$A + B \to P + Q \quad (\text{resp. } P + Q \to A + B).$$

We easily show that global existence of classical solutions does exist in this particular case. For instance, if $\alpha = 0$, the equation

$$\partial_t a - d_a \Delta a = -k_1 ab \leqslant 0$$

implies, by maximum principle, that $|a(t)|_\infty \leqslant |a_0|_\infty$ for all $t \geqslant 0$ and similarly for $b(t)$. This implies that $p, q \in L^\infty(Q_T)$ for all $T > 0$ and that the solutions are classical. However, we are not able to prove that uniform bounds on Q_T are preserved as $k \to +\infty$ although they hold for all k and in the limit as well.

If $\alpha \in (0, 1)$, the limit-reaction is reversible. It is known that, in this case, there is an entropy inequality, like there is also one for the initial reversible system (1). *We prove also here* (*see Theorem* 3) *that this entropy inequality is uniformly preserved along the limit process* $k \to +\infty$. This provides an estimate of $a \ln a$ in $L^2(Q_T)$, which is *uniform in* k_2, k_3 (and not only of a itself), and similarly for b, p, q (see Section 4). This could also be used to pass to the limit in the system, since it provides the uniform integrability of the nonlinear terms, uniformly in k_2, k_3. This $(L\,Log\,L)^2$-approach has been employed in [5]: they prove $L^1(Q_T)$-convergence of a subsequence in the particular case where *the intermediate is initially zero, i.e.* $c(0,\cdot) = 0$. The situation is quite more difficult when $c(0,\cdot) \not\equiv 0$: indeed, a boundary layer appears at $t = 0$ and the mass of c_0 contributes to the mass of the other species. Besides treating this general situation (with bounded initial data), we even prove the *strong* L^2*-convergence* of the solution. It is interesting to notice that we do it independently of the entropy-inequality and in a rather simple way. Moreover, our approach does cover the limit cases $\alpha = 0$, $\alpha = 1$ and independent variations of k_2, k_3 as well: it is very likely that it may be extended to quite general quadratic systems. To end the comparison with [5], let us also emphasize that we prove existence of global *strong*, rather than weak, solutions to the initial system.

2. Proof of Theorem 1

Notations. For $z \in L^r(\Omega)$, $w \in L^r(Q_t)$, $r \in [1,+\infty)$, $t > 0$, we denote

$$|z|_r = \left\{ \int_\Omega |z(x)|^r \, dx \right\}^{1/r}, \qquad |w|_{r,t} = \left\{ \int_0^t \int_\Omega |w(s,x)|^r \, ds\, dx \right\}^{1/r}.$$

The following lemma is inspired from the L^p-duality technique introduced in [19] and generalized to various situations for instance in [22,23,14]. The following version, involving three functions, allows to treat systems like (1) where none of the components is trivially a priori bounded in $L^\infty(Q_T)$ or in $L^p(Q_T)$ for p large.

Lemma 1. *Let u, v, w be regular (in the sense of (3)) with $u \geqslant 0$ and satisfy*

$$\begin{cases} \partial_t u - d_u \Delta u \leqslant \theta_1(\partial_t v - d_v \Delta v) + \theta_2(\partial_t w - d_w \Delta w) & \text{on } Q_T, \\ \partial_n u = \partial_n v = \partial_n w = 0, \end{cases} \tag{7}$$

where $d_u > 0$, $d_v, d_w \in \mathbb{R}$, $\theta_1, \theta_2 \in \mathbb{R}$. Let $r \in (1,+\infty)$. Then, there exists $C = C(T, r, d_u, d_v, d_w, \theta_1, \theta_2)$ such that, for all $t \in [0,T]$,

$$|u|_{r,t} \leqslant C\big[|u(0)|_r + |v(0)|_r + |w(0)|_r + |v|_{r,t} + |w|_{r,t}\big]. \tag{8}$$

Proof. Let $\Theta \in C_0^\infty(Q_T)$ with $\Theta \geqslant 0$, and let ψ be the classical (and nonnegative) solution of

$$-[\partial_t \psi + d_u \Delta \psi] = \Theta, \qquad \frac{\partial u}{\partial n} = 0, \qquad \psi(T) = 0.$$

Multiplying (7) by ψ ($\geqslant 0$) and integrating by parts leads to

$$\begin{cases} \displaystyle\int_{Q_t} u\Theta \leqslant \int_\Omega \psi(0)\big[u(0) - \theta_1 v(0) - \theta_2 w(0)\big] \\ \displaystyle\quad + \int_{Q_t} \Theta[\theta_1 v + \theta_2 w] + \Delta\psi\big[\theta_1(d_u - d_v)v + \theta_2(d_u - d_w)w\big]. \end{cases}$$

We now use the following $L^{r'}$-regularity estimates on ψ (see, e.g., [21]):

Lemma 2. *Let $r' = r/(r-1)$. There exists $C = C(T, d_u, r)$ such that*

$$\forall t \in [0,T], \quad |\partial_t \psi|_{r',t} + |\Delta\psi|_{r',t} + |\psi(0)|_{r'} \leqslant C|\Theta|_{r',t}.$$

We then apply the Hölder inequality in the inequality above together with these estimates to obtain,

$$\int_{Q_t} u\Theta \leqslant C|\Theta|_{r',t}\big[|u(0)|_r + |v(0)|_r + |w(0)|_r + |v|_{r,t} + |w|_{r,t}\big].$$

The estimate (8) follows by duality, with a constant C as announced. $\square$

Remark. For a proof of Lemma 2 see, e.g., [21] where we find it explicitly for $t = T$. Knowing it for $t = T$ and applying it with Θ replaced by $\Theta\chi_{[0,t]}$ will give all the above inequalities.

Proof of Theorem 1. Since the initial data is in $L^\infty(\Omega)$, there exists a classical solution to (1) on a maximal interval $(0, T^*)$ (see Lemma 7 in Appendix A). Moreover, due to the quasi-positivity of the nonlinearities (see again Lemma 7), all components of this solution are nonnegative. To obtain that $T^* = +\infty$, let us prove that, if $T^* < +\infty$, then the solution is uniformly bounded on $[0, T^*) \times \Omega$ which will provide a contradiction (see Lemma 7).

Let us first prove that if $T^* < +\infty$ we have, for all $r \in (1,+\infty)$,

$$|a|_{r,T^*} + |b|_{r,T^*} + |c|_{r,T^*} + |p|_{r,T^*} + |q|_{r,T^*} < +\infty. \tag{9}$$

Then, going back to each equation and applying it with r large enough ($r > 2(N+1)$, say) will imply that a, b, c, p, q are bounded in $L^\infty(Q_{T^*})$ (see, e.g., [21]), whence a contradiction with $T^* < +\infty$.

We assume $T^* < +\infty$ and we denote by C any constant depending on the data, including the L^∞-norm of the initial data and also T^*. By negativity of $-k_1 ab$, we may write

$$\left|a(t)\right|_r \leqslant |a_0|_r + k_2 \int_0^t \left|c(s)\right|_r ds \leqslant |a_0|_r + k_2 \left(T^*\right)^{1/r'} |c|_{r,t}.$$

Similarly:

$$\left|p(t)\right|_r \leqslant |p_0|_r + k_3 \left(T^*\right)^{1/r'} |c|_{r,t}.$$

Now, we apply Lemma 1 with $u = c$, $v = a$, $w = p$ according to the following identity

$$\partial_t c - d_c \Delta c = -(\partial_t a - d_a \Delta a) - (\partial_t p - d_p \Delta p).$$

Then,

$$|c|_{r,t} \leqslant C\left[1 + |a|_{r,t} + |p|_{r,t}\right].$$

Coupling this inequality with the two previous ones, we obtain (with another constant C depending also on k_2, k_3)

$$\left|a(t)\right|_r + \left|p(t)\right|_r \leqslant C\left[1 + |a|_{r,t} + |p|_{r,t}\right] \leqslant C\left[1 + 2g(t)\right],$$

where we denote $g(t) = \{\int_0^t |a(s)|_r^r + |p(s)|_r^r\}^{1/r}$. This gives the following differential inequality for g (again with another constant C):

$$g'(t) \leqslant C\left[1 + g(t)\right].$$

It follows from Gronwall's lemma that g is bounded in $L^\infty(0, T^*)$, and so are $|a(t)|_{r,T^*}$, $|p(t)|_{r,T^*}$, $|c(t)|_{r,T^*}$. Going back to the system, we similarly deduce that $|b(t)|_{r,T^*}$, $|q(t)|_{r,T^*}$ are bounded. This proves (9). □

3. Proof of Theorem 2

Here, we denote by C any constant depending on the data including the L^∞-norm of the initial data, *but not on* k_2, k_3, and by $C(T)$ if it moreover depends on each T.

Let us first prove a series of estimates on the global solution of (1), independently of k_2, k_3. The first one states that we may obtain L^∞-bounds, independently of k_2, k_3, on some small interval $(0, \delta)$ (also independent of k_2, k_3).

Lemma 3. *Let (a, b, c, p, q) be the solution of (1) on $(0, +\infty)$. Then, there exists $\delta > 0$, $C > 0$ independent of k_2, k_3 such that*

$$\sup_{t\in[0,\delta]} \left(\left|a(t)\right|_\infty + \left|b(t)\right|_\infty + \left|c(t)\right|_\infty + \left|p(t)\right|_\infty + \left|q(t)\right|_\infty\right) \leqslant C.$$

Proof. We use the fact that the solution of (1) is bounded above by the solution of the "smallest quasi-monotone o.d.e. above the given system", namely

$$\begin{cases} \partial_t \mathcal{A} = k_2 \mathcal{C}, \\ \partial_t \mathcal{B} = k_2 \mathcal{C}, \\ \partial_t \mathcal{C} = k_1 \mathcal{A}\mathcal{B} - (k_2 + k_3)\mathcal{C} + k_4 \mathcal{P}\mathcal{Q}, \\ \partial_t \mathcal{P} = k_3 \mathcal{C}, \\ \partial_t \mathcal{Q} = k_3 \mathcal{C}, \\ \mathcal{A}(0) = |a_0|_\infty, \quad \mathcal{B}(0) = |b_0|_\infty, \quad \mathcal{C}(0) = |c_0|_\infty, \quad \mathcal{P}(0) = |p_0|_\infty, \quad \mathcal{Q}(0) = |q_0|_\infty. \end{cases} \tag{10}$$

The fact that

$$a \leqslant \mathcal{A}, \qquad b \leqslant \mathcal{B}, \qquad c \leqslant \mathcal{C}, \qquad p \leqslant \mathcal{P}, \qquad q \leqslant \mathcal{Q} \tag{11}$$

is more or less classical (see, e.g., Section 4 in [6]). Let us briefly recall how this may be proved here: if we denote $\bar{a} = \mathcal{A} - a$, $\bar{b} = \mathcal{B} - b$, etc., then we easily check that

$$\begin{cases} \partial_t \bar{a} - d_a \Delta \bar{a} \geqslant k_2 \bar{c}, \\ \partial_t \bar{b} - d_b \Delta \bar{b} \geqslant k_2 \bar{c}, \\ \partial_t \bar{c} - d_c \Delta \bar{c} = k_1\left[(a + \bar{a})(b + \bar{b}) - ab\right] - (k_2 + k_3)\bar{c} + k_4\left[(p + \bar{p})(q + \bar{q}) - pq\right], \\ \partial_t \bar{p} - d_p \Delta \bar{p} \geqslant k_3 \bar{c}, \\ \partial_t \bar{q} - d_q \Delta \bar{q} \geqslant k_3 \bar{c}, \end{cases}$$

together with homogeneous Neumann boundary conditions. The nonlinearity on the right-hand side of this system is quasi-positive (see Lemma 7) so that its solution remains nonnegative for all time since it is initially nonnegative, whence (11).

Now if we set $\mathcal{S} = \mathcal{A} + \mathcal{B} + 2\mathcal{C} + \mathcal{P} + \mathcal{Q}$ in the system (10), we see that

$$\partial_t \mathcal{S} = 2k_1 \mathcal{A}\mathcal{B} + 2k_4 \mathcal{P}\mathcal{Q} \leqslant K\mathcal{S}^2 \quad \text{with } K = k_1 + k_4.$$

It follows that

$$\forall t \in \big(0, \big[\mathcal{S}(0)K\big]^{-1}\big), \quad \mathcal{S}(t) \leqslant \mathcal{S}(0)\big[1 - \mathcal{S}(0)Kt\big]^{-1},$$

and the conclusion of Lemma 3 follows. □

Remark. In case of bounded initial values, uniform bounds are of course always available on small time intervals. The point here is that these bounds are independent of the decay rates of the intermediate. This is not restricted to the case of one intermediate. In fact, the same argument applies to more complex reaction networks with several fast intermediates, given that each transition complex is made of a single component. In this case, and with mass action kinetics, the decay terms in the balance equations of all intermediates remain while passing to the smallest larger quasi-monotone system. This fact then allows to compensate the intermediates' growth terms in the other equations of the comparison system by using appropriate linear combinations of all equations.

Lemma 4. *Let (a, b, c, p, q) be the solution of (1) on $(0, +\infty)$. Then*

$$\forall t \in [0, +\infty), \quad \big|a(t)\big|_1 + \big|b(t)\big|_1 + \big|c(t)\big|_1 + \big|p(t)\big|_1 + \big|q(t)\big|_1 \leqslant C, \tag{12}$$

and for all $T < +\infty$ it holds that

$$|a|_{2,T} + |b|_{2,T} + |c|_{2,T} + |p|_{2,T} + |q|_{2,T} \leqslant C(T), \tag{13}$$

$$(k_2 + k_3) \int_{Q_T} c \leqslant C(T). \tag{14}$$

Proof. Summation of the five equations, the third one taken twice, leads to

$$\partial_t(a + b + 2c + p + q) - \Delta(d_a a + d_b b + 2d_c c + d_p p + d_q q) = 0.$$

Integrating on Ω, then on $(0, t)$, and using the nonnegativity of all components, we obtain (12).

Then, we set

$$W = a + b + 2c + p + q, \qquad Z = d_a a + d_b b + 2d_c c + d_p p + d_q q, \qquad A = Z/W,$$

so that

$$\partial_t W - \Delta Z = 0, \quad \text{or} \quad \partial_t W - \Delta(AW) = 0. \tag{15}$$

Now note that

$$0 < \sigma := \min\{d_a, d_b, d_c, d_p, d_q\} \leqslant A \leqslant \Sigma := \max\{d_a, d_b, d_c, d_p, d_q\} < +\infty. \tag{16}$$

It is known (see [26,27,11]) that this implies L^2-estimates on W. Let us reprove it here more directly, using the simple structure above. We multiply the integrated form of (15), namely

$$W(t) - W(0) - \Delta \int_0^t Z(s)\,ds = 0,$$

by $Z(t)$. We then integrate on Ω and, after integration by parts, we obtain

$$\int_\Omega Z(t)\big[W(t) - W(0)\big] + \int_\Omega \nabla Z(t) \int_0^t \nabla Z(s)\,ds = 0.$$

Integrating this with respect to t on $(0, T)$ gives

$$\int_{Q_T} ZW + \int_\Omega \frac{1}{2}\left|\int_0^T \nabla Z(s)\,ds\right|^2 = \int_{Q_T} ZW(0) \leqslant \sqrt{T}|Z|_{2,T}\big|W(0)\big|_2. \tag{17}$$

Since $W \geqslant \sigma Z$ as indicated in (16), we deduce a bound for Z (and for W) in $L^2(Q_T)$. The estimate (13) follows since all components are nonnegative.

If we integrate the third equation of (1) (i.e. the equation on the component c), we have, using also Schwarz's inequality

$$\int_\Omega c(t) + \int_{Q_t} (k_2 + k_3)c \leqslant \int_\Omega c_0 + k_1 |a|_{2,t} |b|_{2,t} + k_4 |p|_{2,t} |q|_{2,t}.$$

Using also (13), this gives (14). □

We will also use the following result for the proof of Theorem 2. It is more or less classical, but we indicate a proof in Appendix A.

Lemma 5. *Let $d > 0$. The mapping $(w_0, \Theta) \to w$, where w is the solution of*

$$w_t - d\Delta w = \Theta, \qquad \partial_n w = 0 \quad \text{on } \partial\Omega, \qquad w(0,\cdot) = w_0,$$

is compact from $L^1(\Omega) \times L^1(Q_T)$ into $L^1(Q_T)$, even into $L^1((0,T); W^{1,1}(\Omega))$.

Proof of Theorem 2. By (13), the right-hand side of (1) is bounded in $L^1(Q_T)$ for all $T > 0$. By the compactness stated in Lemma 5, and by a diagonal extraction procedure, we may assume that, up to a subsequence, $(U_k, \nabla U_k)$ converges for all $T > 0$ in $L^1(Q_T)^5 \times [L^1(Q_T)^N]^5$ and a.e. on Q_T to a limit function $(U, \nabla U) = ((a,b,c,p,q), (\nabla a, \nabla b, \nabla c, \nabla p, \nabla q))$.

For all $\psi \in \mathcal{C}^\infty([0,T] \times \overline{\Omega})$ with $\psi(T) = 0$ we have

$$\int_{Q_T} \psi(-k_1 a_k b_k + k_2 c_k) + \int_\Omega \psi(0) a_k(0) = \int_{Q_T} -\partial_t \psi a_k + d_a \nabla\psi \nabla a_k, \tag{18}$$

$$\int_{Q_T} \psi(k_1 a_k b_k + k_4 p_k q_k - k c_k) + \int_\Omega \psi(0) c_k(0) = \int_{Q_T} -\partial_t \psi c_k + d_c \nabla\psi \nabla c_k \tag{19}$$

and similarly for b_k, p_k, q_k.

By the estimate (14), kc_k is bounded in $L^1(Q_T)$; in particular, c_k and ∇c_k tend to 0 in $L^1(Q_T)$ and $[L^1(Q_T)]^N$. Since U_k is uniformly bounded on Q_δ, the convergence of U_k on Q_δ holds in all $L^p(Q_\delta)$, $1 \leqslant p < +\infty$ (by a.e. convergence and thanks to the dominated convergence theorem). In particular, $a_k b_k$ (resp. $p_k q_k$) converges in $L^1(Q_\delta)$ to ab (resp. pq). We deduce from (19) that, for all $\psi \in \mathcal{C}^\infty([0,\delta] \times \overline{\Omega})$ with $\psi = 0$ on (δ, T),

$$\lim_{k \to +\infty} \int_{Q_\delta} \psi k c_k = \int_{Q_\delta} \psi(k_1 ab + k_4 pq) + \int_\Omega \psi(0) c_0. \tag{20}$$

Going back to (18), and using $k_2/k \to \alpha$, it follows that

$$\int_{Q_\delta} \psi\big[-k_1 \alpha' ab + k_4 \alpha pq\big] + \int_\Omega \psi(0)[a_0 + \alpha c_0] = \int_{Q_\delta} -\partial_t \psi a + d_a \nabla\psi \nabla a. \tag{21}$$

According to Lemma 8 of Appendix A, a is a weak solution on $[0,\delta]$ of

$$\partial_t a - d_a \Delta a = -k_1(1-\alpha)ab + k_4 \alpha pq.$$

Moreover, $a \in C([0,T]; L^1(\Omega))$ and $a(0) = a_0 + \alpha c_0$.

We obtain the expected similar results for b_k, p_k, q_k and their limits b, p, q. Note in particular (and this is what we will mainly use next)

$$a(0) = a_0 + \alpha c_0, \qquad b(0) = b_0 + \alpha c_0, \qquad p(0) = p_0 + \alpha' c_0, \qquad q(0) = q_0 + \alpha' c_0. \tag{22}$$

Now, *let us show that U_k converges in $L^2(Q_T)$*. For this, we go back to the identity (17) where we now indicate the dependence in k, namely

$$\int_{Q_T} Z_k W_k + \frac{1}{2} \int_\Omega \left| \int_0^T \nabla Z_k(s)\, ds \right|^2 = \int_{Q_T} Z_k W_k(0).$$

Up to a subsequence, we may assume that Z_k, W_k converge weakly in $L^2(Q_T)$ (and a.e. as we already know) to $Z = d_a a + d_b b + d_p p + d_q q$, $W = a + b + p + q$ and $\int_0^T \nabla Z_k(s)\, ds$ converges weakly in $L^2(\Omega)$ to $\int_0^T \nabla Z(s)\, ds$. We have

$$\int_{Q_T} ZW \leqslant \liminf_{k\to+\infty} \int_{Q_T} Z_k W_k, \quad \int_\Omega \left| \int_0^T \nabla Z(s)\,ds \right|^2 \leqslant \liminf_{k\to+\infty} \int_\Omega \left| \int_0^T \nabla Z_k(s)\,ds \right|^2 \tag{23}$$

the first inequality coming for instance from Fatou's lemma and the second one from the weak L^2-convergence. It follows that

$$\int_{Q_T} ZW + \frac{1}{2} \int_\Omega \left| \int_0^T \nabla Z(s)\,ds \right|^2 \leqslant \lim_{k\to+\infty} \int_{Q_T} Z_k W_k(0) = \int_{Q_T} Z\overline{W}_0, \tag{24}$$

with $W_k(0) = \overline{W}_0 := [a_0 + b_0 + 2c_0 + p_0 + q_0]$. Furthermore, we have $W(0) = \overline{W}_0$ according to (22).

Now, we may pass to the limit in the sum of the four equations of type (18) in a_k, b_k, p_k, q_k and of twice Eq. (19) in c_k, namely, for all $\psi \in C^\infty([0,T) \times \overline{\Omega})$ with $\psi(T) = 0$, and, by density, for all $\psi \in C^2([0,T) \times \overline{\Omega})$ with $\psi(T) = 0$,

$$\int_{Q_T} -\partial_t \psi W_k + \nabla\psi \nabla Z_k = \int_\Omega \psi(0) W_k(0) \tag{25}$$

and we obtain in the limit

$$\int_{Q_T} -\partial_t \psi W + \nabla\psi \nabla Z = \int_\Omega \psi(0)\overline{W}_0. \tag{26}$$

We may choose $\psi = \psi_k = \int_t^T Z_k(s)\,ds$ in (26) and similarly choose $\psi = \int_t^T Z(s)\,ds \in W^{1,2}(Q_T)$ in (25) (this is allowed by density) to obtain

$$\int_{Q_T} Z_k W + Z W_k + \int_\Omega \left[\int_0^T \nabla Z_k(s)\,ds \right] \left[\int_0^T \nabla Z(s)\,ds \right] = \int_\Omega \left[\psi_k(0) + \psi(0)\right] \overline{W}_0.$$

Passing to the limit as $k \to \infty$ and using the appropriate weak-L^2 convergence lead to

$$\int_{Q_T} ZW + \frac{1}{2} \int_\Omega \left| \int_0^T \nabla Z(s)\,ds \right|^2 = \int_{Q_T} ZW(0) = \int_{Q_T} Z\overline{W}_0. \tag{27}$$

It follows that *equality holds in* (24) *and therefore also in* (23). In particular, $\int_{Q_T} ZW = \lim_{k\to+\infty} Z_k W_k$. This implies that the convergence of W_k, Z_k is strong (and not only weak) in $L^2(Q_T)$. Indeed, we also know that $A_k = Z_k/W_k$ converges to $A = Z/W$ a.e. on Q_T together with (see (16)) $0 < \sigma \leqslant A_k \leqslant \Sigma < +\infty$. Hence the strong convergence follows from

$$\lim_{k\to+\infty} \int_{Q_T} A_k [W_k - W]^2 = \lim_{k\to+\infty} \int_{Q_T} Z_k W_k - 2 Z_k W + A_k W^2 = 0.$$

Since all functions a_k, b_k, c_k, p_k, q_k are bounded above by W_k, according to the dominated convergence theorem (in its extended version, see $(*)$ below), they also converge strongly in $L^2(Q_T)$. In particular, $a_k b_k$ (resp. $p_k q_k$) converge to ab (resp. pq) in $L^1(Q_T)$ (and not only in $L^1(Q_\delta)$).

Now, we deduce that (20) and (21) hold on Q_T for all $\psi \in C^\infty([0,T] \times \overline{\Omega})$ with $\psi(T) = 0$ (and not only for those ψ with $\psi \equiv 0$ on $[\delta, T]$), and similarly for b, p, q. This completes the proof of Theorem 2.

$(*)$ We obtain it by applying Fatou's lemma to the nonnegative function $(a + W_k)^2 - |a_k - a|^2$ and similarly for the other functions. □

Remark. The solutions U_k of the original RD-systems with finite k are classical solutions, hence, in particular, they belong to $C([0,T], X)$ with $X = L^1(\Omega; \mathbb{R}^5)$. In the general case, we cannot expect convergence in the latter space, since a boundary layer builds up near $t = 0$. But, given a sequence (U_k) for $k := k_2 + k_3 \to \infty$, Theorem 2 yields a subsequence (U_{k_l}) such that $U_{k_l} \to U = (a, b, 0, p, q)$ in $L^2(Q_T)$. Actually, using the approach in [4] and [7], it is possible to prove that $U_{k_l} \to U$ in $C([\tau, T], X)$ for any $\tau > 0$.

4. $[L\,Log\,L]^2$-estimates

Hereafter, we assume that $\alpha \in (0,1)$. We will use the entropy inequality to improve the $L^2(Q_T)$-estimate on the components. We denote by $C(T)$ any constant which does not depend on k_2, k_3 (but depends on the data and on T).

Theorem 3. *Assume* (2) *and* (4) *with* $\alpha \in (0,1)$. *Then, for all* $T > 0$,

$$|a \ln a|_{2,T} + |b \ln b|_{2,T} + |c \ln c|_{2,T} + |p \ln p|_{2,T} + |q \ln q|_{2,T} \leqslant C(T). \tag{28}$$

Proof. We use the *entropy of the system*. We introduce

$$a_1 = b_1 = \sqrt{\frac{k_2 + k_3}{k_3 k_1}}, \qquad p_1 = q_1 = \sqrt{\frac{k_2 + k_3}{k_2 k_4}}, \qquad c_1 = \frac{k_2 + k_3}{k_2 k_3}.$$

Note that,

$$\text{as } k_2 + k_3 \to +\infty: \quad a_1 \to \big[k_1(1-\alpha)\big]^{-1/2}, \qquad p_1 \to [k_4\alpha]^{-1/2}, \qquad c_1 \to 0. \tag{29}$$

We also introduce:

$$w_a = a \ln \frac{a}{a_1} - (a - a_1), \qquad w_b = b \ln \frac{b}{b_1} - (b - b_1), \qquad w_c = c \ln \frac{c}{c_1} - (c - c_1),$$
$$w_p = p \ln \frac{p}{p_1} - (p - p_1), \qquad w_q = q \ln \frac{q}{q_1} - (q - q_1).$$

Recall that $x \ln(x/y) - (x - y) \geqslant 0$ for all $x, y > 0$ with equality at $x = y$. All the functions w_i are nonnegative and we have

$$\partial_t w_a - d_a \Delta w_a \leqslant \ln \frac{a}{a_1}[-k_1 ab + k_2 c],$$

and similarly for w_b, w_c, w_p, w_q. We set

$$W_l = w_a + w_b + w_c + w_p + w_q, \; Z_l = d_a w_a + d_b w_b + d_c w_c + d_p w_p + d_q w_q$$

so that $\partial_t W_l - \Delta Z_l$ is bounded above by

$$[-k_1 ab + k_2 c] \ln \frac{ab}{a_1 b_1} + \big[k_1 ab - (k_2 + k_3)c + k_4 pq\big] \ln \frac{c}{c_1} + [-k_4 pq + k_3 c] \ln \frac{pq}{p_1 q_1}.$$

This is nonpositive since it is equal to the sum of the two following terms:

$$[-k_1 ab + k_2 c]\left[\ln\left(\frac{k_3}{k_2 + k_3}(k_1 ab)\right) - \ln\left(\frac{k_3}{k_2 + k_3}(k_2 c)\right)\right] \leqslant 0,$$
$$[-k_4 pq + k_3 c]\left[\ln\left(\frac{k_2}{k_2 + k_3}(k_4 pq)\right) - \ln\left(\frac{k_2}{k_2 + k_3}(k_3 c)\right)\right] \leqslant 0.$$

Therefore, as for W, Z, we have for all $0 \leqslant \tau \leqslant t$,

$$W_l(t) - W_l(\tau) - \Delta \int_\tau^t Z_l(s)\, ds \leqslant 0.$$

After multiplying by $Z_l(t)$ and integrating on $Q_{\tau,T} = [\tau, T] \times \Omega$ this implies

$$\int_{Q_{\tau,T}} Z_l W_l + \frac{1}{2} \int_\Omega \left[\int_\tau^T \nabla Z_l(s)\, ds\right]^2 = \int_{Q_{\tau,T}} Z_l W_l(\tau).$$

Together with

$$0 < \sigma \leqslant W_l / Z_l \leqslant \Sigma < +\infty$$

it follows that W_l, Z_l are also bounded in $L^2([\tau, T] \times \Omega)$ independently of k_2, k_3 (by the same the proof as for W, Z) if $w_a(\tau), w_b(\tau), w_c(\tau), w_p(\tau), w_q(\tau)$ are bounded in $L^2(\Omega)$ independently of k_2, k_3. According to Lemma 3 and to (29), except may be for $w_c(\tau)$, they are even bounded in $L^\infty(\Omega)$ independently of k_2, k_3 for all $\tau \in [0, \delta]$.

If $c_0 \equiv 0$, then $w_c(0) = c_1$ is bounded in L^∞ independently of k_2, k_3. In this case we can directly deduce (choosing $\tau = 0$) that W_l is bounded in $L^2(Q_T)$.

If $c_0 \not\equiv 0$, since $c_1 \to 0$ as $k = k_2 + k_3 \to +\infty$ (see (29)), then $w_c(0)$ is not bounded, due to the term $\ln c_1$. Actually, as $c(t)$ is expected to tend to zero for $t > 0$, there is a boundary layer at $t = 0$ and more work needs to be done here. We will use Lemma 3 again: let us first verify that $w_c(\delta)$ is bounded in $L^\infty(\Omega)$ independently of k_2, k_3. Since $c(\delta)$ itself is bounded in $L^\infty(\Omega)$, it is sufficient to show the following for some C independent of k_2, k_3:

$$\left|c(\delta)\ln c_1\right|_\infty \leqslant C. \tag{30}$$

Going back to the third equation of (1) in c and using that a, b, p, q are uniformly bounded on $[0, \delta]$ (see Lemma 3), we obtain

$$\forall t \in [0,\delta], \quad \partial_t\left[e^{kt}c\right] - d_c\Delta\left[e^{kt}c\right] \leqslant Ce^{kt},$$

which implies

$$e^{kt}\left|c(t)\right|_\infty \leqslant |c_0|_\infty + C\int_0^t e^{ks}\,ds = |c_0|_\infty + C\left[e^{kt} - 1\right]/k.$$

It follows that

$$\left|c(\delta)\right|_\infty \leqslant \gamma_k := e^{-k\delta}|c_0|_\infty + C/k.$$

The estimate (30) follows since $|[\ln c_1]\gamma_k| \leqslant [\ln k]\gamma_k$ is bounded independently of k_2, k_3.

We have thus proved that W_l is bounded independently of k_2, k_3 in $L^2(Q_{\delta,T})$. By nonnegativity, so are all w_i's. We finally deduce that

$$a\ln a, \quad b\ln b, \quad c\ln c, \quad p\ln p, \quad q\ln q$$

are also bounded in $L^2(Q_{\delta,T})$. Since they are uniformly bounded on $[0, \delta]$, this completes the proof of Theorem 3. $\square$

Remarks. (i) For zero initial value of the intermediate, i.e. for $c(0,\cdot) = 0$, Theorem 3 has essentially been proven in [5].

(ii) The estimate of Theorem 3 proves that $a_k b_k$ and $p_k q_k$ are not only bounded in $L^1(Q_T)$, but even uniformly integrable on Q_T. This, coupled with their a.e. convergence, gives an alternative proof of their strong $L^1(Q_T)$-convergence to ab, pq, by using the following lemma:

Lemma 6 *(Vitali). Let (f_n) be a sequence of functions bounded in $L^1(Q_T)$ such that*

- *f_n converges a.e. to some f,*
- *(f_n) is uniformly integrable or, equivalently, $\int_{Q_T} \Phi(|f_n|) < +\infty$ for some $\Phi : \mathbb{R}_+ \to \mathbb{R}$ with $\lim_{r\to+\infty} \Phi(r)/r = +\infty$.*

Then f_n converges in $L^1(Q_T)$ to f.

5. Summary

Let us summarize the new results presented in this paper concerning the prototype reaction–diffusion system modeling the reversible chemical reaction

$$A + B \rightleftharpoons C \rightleftharpoons P + Q$$

when the decay of C into the products P and Q, or back to the educts A and B, is extremely fast.

First, we prove global existence in time of *bounded classical solutions – and not only weak solutions* – for the system modeling the above reaction according to the mass action law.

As the main new result we prove that, as one or both of the decay rates of the intermediate component C tend to $+\infty$, the solutions of the initial system converge in $L^2(Q_T)$ to the *weak* solutions of the expected limit system given by the usual quasi-steady-state approach. We emphasize that this is done for all bounded initial data, including the case when the initial mass of C is not zero (where boundary layers appear at $t = 0$). The convergence is obtained in the natural space L^2; the proof is new and exploits very efficiently the L^2-a priori estimates valid for systems for which nonlinear reactive terms add up to a nonpositive sum.

Using the entropy inequality, well-known for these reversible systems, it is also proved, again for all bounded initial data, that the solutions are bounded in $[L\,Log\,L]^2$ independently of the decay rates of C (it was known before only for zero C-initial mass). This gives an alternative proof of the L^2-convergence result, but it is important to notice that this entropy inequality was not needed for the proof of the latter. This allows for instance to include in the same proof the appearance of nonreversible reactions in the limit. It would be interesting to identify the family of quadratic systems to which this approach carries over, knowing in particular that the entropy structure is no longer needed.

Note added to the summary: let us mention some very recent progress on these questions. The L^2-compactness of the U_k in Theorem 2 could actually be proved without the help of Lemma 3 and even for L^2-initial data (see [10,24]). However, Lemma 3 is needed for the above proof of the $L\,Log\,L$ estimate.

Appendix A

Let us first recall the classical local existence result for reaction–diffusion systems of type (1) (see e.g. [18,28,1]):

Lemma 7. *Let us consider the following $m \times m$ system: for all $i = 1, \dots, m$,*

$$\partial_t u_i - d_i \Delta u_i = f_i(u_1, \dots, u_m), \qquad \partial_n u_i = 0 \quad \text{on } \partial\Omega, \qquad u_i(0) = u_{i0}, \tag{31}$$

where $d_i \in (0, +\infty)$, $f_i : \mathbb{R}^m \to \mathbb{R}^m$ is C^1 and $u_{i0} \in L^\infty(\Omega)$. Then, there exists $T > 0$ and a unique classical solution of (31) on $[0, T)$. If T^* denotes the greatest of these T's, then

$$\Big[\sup_{t \in [0,T^*), 1 \leqslant i \leqslant m} \big\|u_i(t)\big\|_{L^\infty(\Omega)} < +\infty\Big] \quad \Rightarrow \quad \big[T^* = +\infty\big]. \tag{32}$$

If, moreover, the nonlinearity $(f_i)_{1 \leqslant i \leqslant m}$ is quasi-positive *which means*

$$\forall i = 1, \dots, m,\ \forall u_1, \dots, u_m \geqslant 0, \quad f_i(u_1, \dots, u_{i-1}, 0, u_{i+1}, \dots, u_m) \geqslant 0,$$

then

$$[\forall i = 1, \dots, m,\ u_{i0} \geqslant 0] \quad \Rightarrow \quad \big[\forall i = 1, \dots, m,\ \forall t \in \big[0, T^*\big),\ u_i(t) \geqslant 0\big].$$

Remark. According to (32), in order to prove global existence of classical solutions for a system like (31), it is sufficient to prove that, if $T^* < +\infty$, then the solutions u_i are uniformly bounded on $[0, T^*)$.

Proof of Lemma 5. *Preliminary remark*: Recall that the Sobolev space $W^{1,1}(\Omega)$ is equipped with the norm $\|v\|_{W^{1,1}} = |v|_1 + |\nabla v|_1$. Thus, convergence in $L^1((0,T); W^{1,1}(\Omega))$ is equivalent to convergence of functions together with their gradients in $L^1(Q_T)$.

We may obtain the result of Lemma 5 by duality as done in [3] in the case of homogeneous Dirichlet boundary conditions. The adjoint of the operator $\mathcal{T} : (w_0, \Theta) \to (w, \nabla w)$ is defined through the mapping

$$\mathcal{T}^* : (\Phi_i)_{0 \leqslant i \leqslant N} \in C_0^\infty(Q_T) \to \big(z(0), z\big),$$

where z is the solution of

$$-\partial_t z - d\Delta z = \Phi_0 - \sum_{1 \leqslant i \leqslant N} \partial_{x_i} \Phi_i, \qquad \frac{\partial z}{\partial n} = 0 \quad \text{on } \partial\Omega, \qquad z(T) = 0.$$

Indeed, if $\Phi = (\Phi_i)_{1 \leqslant i \leqslant N}$,

$$\int_{Q_T} w\Phi_0 + \nabla w \cdot \Phi = \int_{Q_T} -w[\partial_t z + \Delta z] = \int_{\Omega} z(0) w_0 + \int_{Q_T} z\Theta,$$

that is

$$\big\langle \mathcal{T}(w_0, \Theta), (\Phi_0, \Phi)\big\rangle = \big\langle (w_0, \Theta), \mathcal{T}^*(\Phi_0, \Phi)\big\rangle.$$

It is known (see, e.g., [21]) that, if $p > \frac{N}{2} + 1$, $q > N + 2$ and $X = L^p(Q_T) \times [L^q(Q_T)]^N$, then, for some small $\alpha > 0$, the $C^\alpha(Q_T)$-Hölder norm of z satisfies

$$\|z\|_{C^\alpha(Q_T)} \leqslant \kappa \big\|(\Phi_0, \Phi)\big\|_X,$$

where κ is a constant depending only on the data (and on the regularity of $\partial\Omega$). By density, $\mathcal{T}^*$ uniquely extends to a continuous operator from X into $C^\alpha(\Omega) \times C^\alpha(Q_T)$ and consequently to a compact operator from X into $L^\infty(\Omega) \times L^\infty(Q_T)$. It follows that $\mathcal{T}$ may be defined as a compact operator from $L^1(\Omega) \times L^1(Q_T)$ into $X' = L^r(Q_T) \times [L^s(Q_T)]^N$ for all $r < (N+2)/N$ and all $s < (N+2)/(N+1)$. Taking $r = s = 1$ yields Lemma 5. $\square$

Lemma 8. *Let $(S(t))_{t\geqslant 0}$ be the semigroup generated by the operator $d\Delta$ with homogeneous Neumann boundary conditions, where $d>0$. Let $(w_0,F)\in L^1(\Omega)\times L^1(Q_T)$. Then,*

$$\forall t\in[0,T],\quad w(t)=S(t)w_0+\int_0^t S(t-s)F(s)\,ds, \tag{33}$$

is equivalent to

$$\left.\begin{aligned} &w\in L^1\big((0,T);W^{1,1}(\Omega)\big),\quad \forall\psi\in\mathcal{C}^\infty\big([0,T]\times\overline{\Omega}\big)\quad \text{with } \psi(T)=0,\\ &\int_{Q_T}-\partial_t\psi\, w+\nabla w\nabla\psi=\int_\Omega \psi(0)w_0+\int_{Q_T}\psi F. \end{aligned}\right\} \tag{34}$$

In particular, any solution of (34) is continuous from $[0,T]$ into $L^1(\Omega)$ and $\lim_{t\to 0+}w(t)=w_0$.

Proof. Let us first recall why (33) implies (34). For regular enough data (w_0,F), the function w given by (33) is a classical solution of

$$\partial_t w-d\Delta w=F,\qquad \partial_n w=0\quad\text{on }\partial\Omega,\qquad w(0)=w_0.$$

We multiply this by ψ to obtain (34). If now $(w_0,F)\in L^1(\Omega)\times L^1(Q_T)$ only, we approximate (w_0,F) by a sequence of regular functions (w_0^n,F^n) for which (34) holds. The corresponding solutions w^n converge in $C([0,T];L^1(\Omega))$ to the function $t\to w(t)=S(t)w_0+\int_0^t S(t-s)F(s)\,ds$. Moreover, as we know for instance from Lemma 5, (w^n) is compact in $L^1((0,T);W^{1,1}(\Omega))$, so that ∇w^n converges in $L^1(Q_T)$ to ∇w. This allows to obtain the identity (34) for w by passing to the limit in the same identity written for w^n.

Now, in order to show that (34) implies (33), it is sufficient to prove uniqueness of the functions w satisfying (34), namely to prove that the following properties:

$$\left.\begin{aligned} &w\in L^1\big((0,T);W^{1,1}(\Omega)\big),\\ &\forall\psi\in\mathcal{C}^\infty\big([0,T)\times\overline{\Omega}\big)\quad\text{with } \psi(T)=0,\quad \int_{Q_T}-\partial_t\psi\, w+\nabla w\nabla\psi=0 \end{aligned}\right\} \tag{35}$$

imply $w\equiv 0$.

For Θ arbitrary in $\mathcal{C}_0^\infty(Q_T)$, we introduce the solution of the dual problem

$$-\partial_t z-\Delta z=\Theta,\qquad \partial_n z=0\quad\text{on }\partial\Omega,\qquad z(T)=0.$$

Note that the relation in (35) extends by density to all $\psi\in C^2(\overline{Q_T})$ with $\psi(T)=0$. It may be applied to $\psi=z$ (which is C^2 since the boundary of Ω is assumed to be regular; $C^{2+\epsilon}$ would be sufficient). Therefore

$$0=\int_{Q_T}-\partial_t z w+\nabla w\nabla z=\int_{Q_T}-\partial_t z w-w\Delta z=\int_{Q_T}\Theta w.$$

The point here is to justify the integration by parts: it is valid since z is C^2 and $\partial z/\partial n=0$ on $\partial\Omega$; indeed, we may first write the integration by parts for regular approximations of w and then pass to the limit. Finally, by arbitrarity of Θ, the property $\int_{Q_T}\Theta w=0$ implies $w\equiv 0$. $\square$

Remark. One has to be careful with the kind of uniqueness property as the one just proved. Just to emphasize that this is not a trivial question, even for the corresponding elliptic version, let us recall that

$$u\in W_0^{1,1}(\Omega),\qquad \Delta u=0\quad\text{in }\Omega$$

does not imply $u\equiv 0$ for a general bounded open set Ω. However it is the case if Ω is regular, and one classical way to prove it is to introduce the dual problem as we did above for the parabolic version and to use the regularity of its solution (which uses the regularity of Ω itself). Note that the stronger property

$$u\in W_0^{1,2}(\Omega),\qquad \Delta u=0\quad\text{in }\Omega$$

does imply $u\equiv 0$ for any bounded open set Ω (the proof is straightforward).

Remark. *About uniqueness of weak solutions of the nonlinear system*. Even in the case of a regular domain Ω, it is not to be expected that weak solutions of the nonlinear system (in the sense of (5)–(6)) are unique. Indeed, it is known that even for the simple equation

$$\partial_t u - \Delta u = u^3, \qquad u = 0 \quad \text{on } \partial\Omega, \qquad u(0) = u_0 \geqslant 0,$$

uniqueness of weak solutions does not hold in general, even for C^∞-initial data u_0 (see [17] and [2]). Uniqueness is valid among uniformly bounded solutions (see Lemma 7 above). But other solutions may exist which are even C^∞ on $(0, T)$ but for which $\lim_{t\to 0+} |u(t)|_\infty = +\infty$ (although u_0 is very regular).

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